Tess Eleonora Smidt

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Education and Training

Lawrence Berkeley Laboratory (Fall 2018 - Present)
Luis W. Alvarez Postdoctoral Fellow

University of California, Berkeley (Fall 2012 - Spring 2018)
Ph.D, Physics Awards Spring 2018
M.A., Physics Awarded Spring 2014
National Science Foundation Research Fellow (GPA: 3.8/4.0)
Advisor: Prof. Jeffrey B. Neaton
Subfield: Computational Condensed Matter Physics

Massachusetts Institute of Technology (Fall 2008 - Spring 2012)
S.B., Physics with minor in Architecture (GPA: 4.5/5.0)
Advisor: Prof. Janet Conrad
Subfield: Experimental and Computational Particle Physics

Research Interests:
Deep learning for science, materials design, procedural geometry

Computing tools: Density functional theory, high-performance computing, Python, scientific workflows, TensorFlow, PyTorch, CAD

Selected Coursework:
Deep Learning, Computational Geometry, Quantum Field Theory

Luis W. Alvarez Postdoctoral Fellow in Computing Sciences (Fall 2018 - Present)

Lawrence Berkeley Laboratory

- ***Awarded two year fellowship to pursue unrestricted, independent research in computational science.***
- ***Designing neural networks to generate novel atomic crystal structures.*** This will alleviate current bottlenecks in high-throughput computational materials discovery pipelines where searches are limited to databases of experimentally known materials.

Google Internship: Accelerated Science Team (Summer 2017 - Spring 2018)

- ***Designed and implemented a 3D-rotation-equivariant convolutional neural network in TensorFlow.*** How to create such a network had been an open question in deep learning for several years. Initiated project within the Accelerated Science team. Network can identify local features in different positions and orientations in 3D using network connectivity and filters that are compatible with representations of the group of 3D rotations. Network can accept scalars, vectors, and tensor fields as input and output. This network can be used to predict properties of molecules and crystals given the coordinates of constituent atoms as input. Model is available on GitHub.
- ***Created machine learning models to predict quantities relevant for catalysis.*** Models interpolate between computationally expensive quantum mechanical calculations performed by academic collaborators. Used variety of model architectures and hyperparameter searches to train models that could predict relevant quantities within an order of magnitude of quantum mechanical calculation accuracy with simple featurization. Identified several data features that impact hydrogen adsorption energy.

Graduate Research

- ***Helped discover two new classes of crystals.*** Worked with synthetic chemists to characterize a new class of self-assembled crystals with exotic 2D optical and electronic properties in a 3D form. Operated one of the world's strongest magnets and most intense x-ray sources to characterize a new

quantum magnetic material. Predicted the stability of a new class of quantum magnetic crystals. Simulated crystal growth using Metropolis-Hastings algorithm.

- ***Performed an automated computational search for ferroelectrics -- materials used for tunable capacitors and non-volatile RAM.*** Integrated crystal structure databases, symmetry tools, workflow software, density functional theory, visualization, and analysis. Workflow and analysis tools contributed to atomate and pymatgen python packages. First dataset of 150 high-quality ferroelectric candidates in preparation for open submission.
- ***Designed algorithms for generating new atomic systems from geometric primitives.*** Created a geometric algorithm to coat curved surfaces with a graphene-like structure using anisotropic Delaunay triangulations. Used geometric models to correlate structural deformations with changes in electronic properties of atoms that form low-dimensional chains of connected polyhedra.
- ***Created tools for improving synthesis reproducibility.*** To augment paper notebooks used by synthesis groups, I created a lab database system to connect material synthesis methods with experimental data.

Undergraduate Research

- Designed a 40'-long light detection system structure for a 70-ton liquid argon neutrino detector. This structure was installed in 2013.
- Designed a new neutrino source. Simulated particle physics, nuclear physics, and heat transfer.
- Conducted preliminary feasibility study of whether a new Higgs boson interaction type could be detected at the Large Hadron Collider.

Mischief

- ***The Lunch Experiment*** -- Developed an automated system that invited grad students from different departments to group lunches. Organized over 150 "randomized controlled lunches" and grew a community of more than 400 grad students from 50 departments. ***(Summer 2015 - Spring 2016)***
- ***Cosmic Ray Chandeliers*** -- Funded by MIT to design, fabricate, and install two 4' tall chandeliers that illuminate upon detecting cosmic ray muons – particles created when nuclei from outer space bombard Earth's atmosphere. See http://www.blondegeek.net/cosmicray/ ***(Fall 2010 - Spring 2011)***
- ***blondegeek.net*** -- Launched t-shirt company in Summer 2006 at age 16. Designed web site, created customer and product databases and wrote inventory management software. During ten years of business, designed and sold thousands of shirts. ***(2006-2016)***

Publications In Preparation

- **T. Smidt**, S. Griffin, J. B. Neaton, *Ab initio Studies of Structural and Energetic Trends in the Harmonic Honeycomb Iridates*, In preparation for submission to Physical Review: B (2020).

Publications and Patent

- **T. Smidt**, S. Reyes-Lillo, A. Jain, J. B. Neaton, *An Automatically Curated First-Principles Database of Ferroelectrics*, Submitted to Nature Scientific Data (2018). Accepted (2020).
- **T. Smidt***, N. Thomas*, et al., Tensor field networks: Translation- and 3D rotation- equivariant convolutional neural networks. arXiv:1802.08219 (2018). **denotes equal contribution*
- Kiran Mathew et al., *Atomate: A High-Level Interface to Generate, Execute, and Analyze Computational Materials Science Workflows*, Computational Materials Science, Volume 139, 140-152 (2017).

- J.N. Hohman, M. Collins, and **T. Smidt**, *Mithrene and methods of fabrication of mithrene*, (2017). International Patent App. PCT/US20l7/045609. Filed August 4, 2017.
- K. Modic, **T. Smidt,** I. Kimchi et al., *Realization of a three-dimensional spin-anisotropic harmonic honeycomb iridate*, Nature Communications 5 (2014). (arXiv:1402.3254)
- T. Briese et al., *Testing of Cryogenic Photomultiplier Tubes for the MicroBooNE Experiment*, Journal of Instrumentation 8, T07005 (2013). (arXiv:1304.0821)
- A. Bungau et al. *Proposal for an electron antineutrino disappearance search using high-rate 8Li production and decay,* Physical Review Letters 109, 141802 (2012). (arXiv:1205.4419)
- A. Bungau, **T. Smidt** et al., *Simulations of Pion Production in the DAEδALUS Target*, Conference proceedings for the International Particle Accelerator Conference (2012). (arXiv:1205.4419)
- L. Bugel et al., *Demonstration of a Lightguide Detector for Liquid Argon TPCs*, Nuclear Instruments and Methods in Physics Research Section A (2011). (arXiv:1101.3013)
- J. Alonso et al., *Expression of Interest for a Novel Search for CP Violation in the Neutrino Sector: DAEdALUS*, (2010). (arXiv:1006.0260)

Awards

- *People's Choice Winner -- Berkeley Lab Research SLAM,* Berkeley Lab, Berkeley, CA (Sept., 2019)
  12 Berkeley Lab postdoc and early career finalists are challenged to present a compelling three minute presentation of their research in a language appropriate to a non-specialist audience in front of a live audience. Competitors are allowed one PowerPoint slide, but no other resources or props. The audience of Berkeley Lab employees at the live event vote for the "People's Choice" winner.
- *Rising Stars in Computational and Data Science,* Oden Institute at UT Austin, Austin, TX (April 2019)
  Selected to participate in an intensive workshop for women graduate students and postdocs who are interested in pursuing academic and research careers. One of 40 participants with an applicant selection rate of 21%. Each participant gave a 12 min talk on her research.

Tutorials

- *E(3) Equivariant Tutorial,* Institute of Pure and Applied Mathematics at UCLA, Los Angeles, CA (Nov. 2019)
  Organized and ran a tutorial on 3D Euclidean symmetry equivariant neural networks. The tutorial consists of lecture and interactive code examples for 20 participants at the IPAM Long Program on the Machine Learning for Physics and the Physics of Learning. See https://blondegeek.github.io/e3nn_tutorial/ for more details.

Software

- *Co-developer of e3nn* https://github.com/e3nn/e3nn (Jan. 2019 - Present)
  Framework for 3D Euclidean symmetry equivariant neural networks.

Invited Conference and Workshop Talks (Upcoming and Previous)

- *CECAM-Lorentz workshop on Computing Complex Mechanical Systems, EPFL,* Lausanne, Switzerland (Jan. 2020)
- *From Passive to Active: Generative and Reinforcement Learning with Physics,* Institute of Pure and Applied Mathematics (IPAM) at UCLA, Los Angeles, CA (Sept. 2019)
- *Machine Learning for Quantum Matter,* Nordita, Stockholm, Sweden (Aug. 2019)
- *CNMS User Meeting,* Oak Ridge National Laboratory, Oak Ridge, TN (Aug. 2019)

- *MolKin 2019: Molecular Kinetics and Sampling, Design and Machine Learning,* Freie Universität Berlin, Berlin, Germany, (June 2019)
- *Machine Learning in Materials Genome,* Anargyrios and Korgialenios School of Spetses, Spetses, Greece (June 2019)
- *Structure in the Micro-world,* TGDA at Ohio State University, Columbus, OH (May 2019)
- *Foundational & Applied Data Science for Molecular and Materials Sci. & Eng.,* I-DISC at Lehigh University, Bethlehem, PA (May 2019)
- *Machine Learning in Nonlinear Physics and Mechanics,* American Physical Society (APS) March Meeting, Boston, MA (March 2019)
- *Molecular and Electronic Structure Theory Meets Data Science Session,* Society for Industrial and Applied Mathematics (SIAM) Computational Science and Engineering Conference, Spokane, WA (March 2019)
- *Machine Learning for Molecules and Materials Workshop,* Conference on Neural Information Processing Systems (NeurIPS), Montreal, Canada (Dec. 2018)
- *ML4Science Workshop,* Lawrence Berkeley Laboratory, Berkeley, CA (Sept. 2018)

Invited Seminars Talks (Upcoming and Previous)

- *Applied Artificial Intelligence Institute (AAII) Seminar,* UC Santa Cruz, Santa Cruz, CA (Apr. 2020)
- *Center for Computing Research Seminar,* Sandia National Laboratory, Albuquerque, NM (Mar. 2020)
- *Distinguished Young Academics Data Scientists (DYADS) Seminar,* eScience Institute at the University of Washington, Seattle, WA (Dec. 2019)
- *Seminar,* Flatiron Institute, New York, NY (May 2019)
- *Deep Learning Group Seminar,* Sandia National Laboratory, Livermore, CA (May 2019)
- *Berkeley Statistics and Machine Learning Discussion Group,* University of California, Berkeley, CA (Nov. 2018)
- *Molecular Foundry Seminar,* Lawrence Berkeley Laboratory, Berkeley, CA (Oct. 2018)

Contributed Talks (Upcoming and Previous)

- *AI & Molecular World Track,*
  Applied Machine Learning Days, EPFL, Lausanne, Switzerland (Jan. 2020)
- *Computational Discovery and Design of Novel Materials Session,*
  American Physical Society (APS) March Meeting, New Orleans, LA (Mar. 2017)
- *Computational Materials Discovery and Design - Electronic Structure Session,*
  American Physical Society (APS) March Meeting, Baltimore, MA (Mar. 2016)
- *Focus Session: Honeycomb and Pyrochlore Lattices*,
  American Physical Society (APS) March Meeting, San Antonio, TX (Mar. 2015)
- *Focus Session: Frustrated Magnets and Spin-Orbit Coupling*,
- American Physical Society (APS) March Meeting, Denver, CO (Mar. 2014)
- *Accelerator Neutrino Experiments Session,*
  American Physical Society (APS) April Meeting, Atlanta, GA (Apr. 2012)

Training

- *UCSF Scientific Leadership and Management Skills Course,* Gladstone Institute at UCSF, San Francisco, CA (May 1 and 8, 2019)
  16 hours of training based on the HHMI publication Making the Right Moves: A Practical Guide to Scientific Management for Postdocs and New Faculty.

Outreach

- *Seminar for Computational Materials at Berkeley*, University of California, Berkeley, Berkeley, CA (Oct. 2018)
- *Penpal for Letters to a Pre-scientist* (Fall 2018 to Spring 2019)
- *Seminar for LBL Computing Sciences Summer Student Series*, Lawrence Berkeley Laboratory, Berkeley, CA (July 2019)

Interns and Advised Students

- Elliott Perryman (BS student at the Univ. of Tennessee at Knoxville and SULI Intern at LBL) (Spring 2020)
- Kostiantyn Lapchevskyi (MA student at Ukrainian Catholic University, advised thesis work) (Fall 2019)
- Mario Geiger (PhD student at EPFL and Summer Intern at LBL) (Summer 2019)
- Ben Miller (MA student at Freie Universität Berlin and Summer Intern at LBL) (Summer 2019)
- Hashim Piracha (BS student at UC Berkeley and Summer Intern at LBL) (Summer 2019)

Professional Service

- *Co-organizer of 2019 Bay Area Scientific Computing Day*, *Lawrence Berkeley Laboratory*, Berkeley, CA (Dec. 16, 2019)
  Annual one-day meeting focused on fostering interactions and collaborations between researchers in the fields of scientific computing and computational science and engineering from the San Francisco Bay Area and nearby regions.
- *Co-organizer of Hands-On sessions of 2020 Berkeley Lab Deep Learning School*, *Lawrence Berkeley Laboratory,* Berkeley, CA (July 20-24, 2020)